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Surface stabilisation of the ferromagnetic phase of $FeGe_2$

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Abstract

Electronic and magnetic properties of bulk and films of $FeGe_2$ are investigated within ab initio density functional theory. Bulk structure displays an anti-ferromagnetic ground state with Fe magnetic moment of $1.36\mu_B$ and a ferromagnetic configuration a few mRy above. Thin films with a few monolayers display a ferromagnetic ground state with a metastable anti-ferromagnetic configuration a few mRy above. A transition from ferromagnetism to anti-ferromagnetism is observed when the thickness of the film is increased. A strong increase of the magnetic moments, up to $2.64\mu_B$, on Fe atoms present at the surface is observed.

Keywords: Iron–Germanium compounds; Magnetic films; Anti-ferromagnetic coupling

1. Introduction

Transport of spin across the ferromagnetic-semiconductor interface and their manipulation has wide implication for spintronic [1]. Therefore many important researches are presently devoted to ferromagnetic semiconductors. The particular interest in Fe–semiconductor systems, like Fe–Ge or Fe–GaAs, is driven by the close lattice match between the two materials enabling growth of single-crystal structure [2]. $FeGe_2$ crystallises with the tetragonal ($C16$) structure ($a = 5.908$ Å and $c = 4.955$ Å) [3]. Its magnetic properties were first studied by Yasukochi et al. [4] who reported anti-ferromagnetic behaviour as well as a weak ferromagnetic component. Later on Kren and Szabo [5] suggested, via neutron diffraction, a collinear anti-ferromagnetic structure. A more complete (temperature-dependent) neutron study was performed by Corliss et al. [6]. They deduced a phase diagram using mean-field and renormalisation group consideration. Vlasov et al. [7] gave a description of the magnetic hysteresis and the field

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dependence of the reversible and irreversible susceptibilities. Also spin-wave damping was pointed out by Adams et al. [8].

On the theoretical side, the bulk magnetic structure of $FeGe_2$ has been calculated by Grechnev et al. [9]. Using local spin density approximation and the augmented spherical wave (ASW) method, they investigated various magnetic configurations where the Fe magnetic moments coupling is ferromagnetic, anti-ferromagnetic and non-collinear. Their results show that the anti-ferromagnetic configuration, having the lowest total energy, is the ground state of the bulk $FeGe_2$. We are not aware of any ab initio calculation concerning the derivation of electronic and magnetic properties of $FeGe_2$ based two-dimensional systems.

However, there are a few calculations concerning Fe/Ge superlattices. Pickett and Papacontantopoulos [11] performed parametrised tight-binding calculations of the Fe/Ge(1 1 0) interface. Butler and co-workers [12] calculated the electronic structure of the spin-dependent tunnelling structures Fe/Ge/Fe. Cabria et al. [13] within Linearised Muffin-tin Orbitals (LMTO) calculation obtained an induced moment of Ge in bcc Fe/Ge superlattices. Those results have been confirmed experimentally, within X-ray Magnetic Circular Dichroism (XMCD) by Freeland et al. [2]. Yamada et al. [14] calculated with LMTO method the electronic structure and magnetism of FeGe with B20-type structure. Later on, Yamada et al. [15] reported on itinerant-electron metamagnetism of Fe(Si,Ge) with B20-type structure. Recently, Perlov et al. [16] presented results on calculations of the electronic, magnetic and transport properties of Fe/Ge multilayered systems. The calculations referred to are certainly interesting but they are performed on different Fe–Ge compounds.

The purpose of the present communication is to present first an ab initio band structure of $FeGe_2$ crystal and second to discuss the magnetic surface reconstruction of a thin slab of $FeGe_2$. Bulk $FeGe_2$ presents an anti-ferromagnetic ground state with a metastable ferromagnetic configuration a few mRy above. However, in thin slabs the situation may appear different and one may expect a relative stabilisation of the ferromagnetic configuration similar to the results obtained by Lounis et al. [18] on FeRh. Within TBLMTO (Tight Binding Linear Muffin-Tin Orbital) calculations, they have shown a transition from ferromagnetic configuration (for thin FeRh slabs) to anti-ferromagnetic configuration for thicker slabs as well as for bulk behaviour. Indeed FeRh is anti-ferromagnetic in the bulk form but a small increase of Fe concentration induces a transition towards ferromagnetism. The difference of energy between the anti-ferromagnetic ground state and the metastable ferromagnetic state in $FeGe_2$ being a few mRy, a possible transition towards ferromagnetism is expected when the thickness of the slab is thin.

Section 2 is devoted to a short outlook of the method used and the results obtained in the case of bulk system. Section 3 is devoted to calculation displaying the magnetisation at the surface of $FeGe_2$ thin films. It is found that the magnetic ground state is determined by both thickness and chemical composition of the spacer, being ferromagnetic for thin and anti-ferromagnetic for thicker films. Discussion and conclusion are reported in Section 4.

2. Computational model and bulk lattice parameter optimisation

The electronic structure calculation and the magnetic configurations of bulk $FeGe_2$, in the $C16$ structure, are investigated within density functional theory. We use the scalar-relativistic tight-binding linear muffin-tin orbital (TB-LMTO) method with the atomic spheres approximation [17]. First we performed calculations on the bulk $FeGe_2$. The von Barth–Hedin local exchange correlation potential is used with the Langreth–Mehl–Hu non-local correction [10]. The eigenvalues and -vectors are determined using the tetrahedron technique with an increasing number of k points in the irreducible Brillouin Zone (BZ), until final convergence is obtained (512 k points are used for bulk calculations and 256 k points for films calculations).

A cell of four types of Fe atoms and eight types of Ge atoms is considered. The iron atoms are located on two plans in alterance with two plans of Ge. A plan of empty spheres is inserted between